MOLECULAR DYNAMICS AND FINITE ELEMENT METHOD BASED MODELLING AND SIMULATIONS OF NANOPARTICLES AND NANOCOMPOSITES FOR ADVANCED STRUCTURAL APPLICATIONS

A Thesis Submitted in Partial Fulfillment of the Requirements
For the Degree of
Doctor of Philosophy

by

KRISHNAN BANDYOPADHYAY
(NITD/PhD/MT/2015/00686)

Under the Supervision
of
DR. M.M. GHOSH
&
PROF. K.S. GHOSH



Department of Metallurgical and Materials Engineering
NATIONAL INSTITUTE OF TECHNOLOGY DURGAPUR
WEST BENGAL – 713209
INDIA

December, 2021

ABSTRACT

Development of new challenging materials with enhanced mechanical and physical properties is the prime concern for advanced structural applications, like in space, defense, navy, nuclear reactor, etc. With advancement of the society vis-à-vis all the different vital sectors, there is ever-increasing demand for new potent structural materials with more and more enhanced mechanical and physical properties. Alloying and nanostructuring are the two well-known ways for enhancing the mechanical properties of metallic materials. However, a complete scheme for designing a promising material for any advanced structural application by means of alteration of alloy composition and/or crystallite size under nanoscale regime is still lacking. Developing a new challenging structural material through only the experimental route needs several experimental trials with associated difficulties. A relatively better and competent way is to designing first the most potent material for any advanced structural application through suitable materials modelling and simulations approach, followed by producing the target material through a suitable experimental route under strict control of experimental parameters.

In the present research, different models have been developed using MD and FEM based multiscale approaches under varying parametric conditions. Simulations of these models have led to the design and development of nanoparticles, nanostructured thin films and nanocomposites with promising mechanical and other physical properties for advanced structural applications. The MD based tensile and compressive models for various pure metal and alloy nanoparticles have yielded engineering stress – strain curves; from which important mechanical properties, viz. yield strength, Young's modulus and %elongation have been estimated under varying compositions. The MD simulations have shown that the nanoparticles have yield strength values several orders of magnitude greater than those of their bulk material counterparts. However, the Young's modulus values of the nanoparticles are only few times greater than those of their bulk material counterparts. The MD based nanoindentation model has been designed following the Oliver and Pharr method of nanoindentation testing. The nanoindentation modelling of both the single crystal and poly-nanocrystalline Cu-Ni alloy thin film with nanoscale film thickness has revealed enhancement of hardness by several orders of magnitude and enhancement of Young's modulus by few (2-3) times only, in comparison with their bulk material counterpart. In Cu-Ni alloy thin

film with nanoscale film thickness hardness is much more sensitive to the predominant surface effect of the thin film than the Young's modulus. The hardness and Young's modulus of single crystal and poly-nanocrystalline Cu-Ni alloy thin film with a given nanoscale film thickness can be altered by altering alloy composition and/or crystallite size. The most potent alloy thin film with nanoscale film thickness can be designed by tuning alloy composition only in case of single crystal structure and both the alloy composition and crystallite size in case of poly-nanocrystalline structure. Apart for MD based tensile/compressive and nanoindentation modelling, a multiscale model has also been developed here which comprises of both MD and FEM techniques for designing the most potent nanocomposite for advanced structural applications. In the multiscale approach, first MD has been used for evaluating the mechanical properties, viz. Young's modulus, hardness and yield strength of nanoparticles under varying compositions and/or crystallite sizes and by tuning these parameters (composition and/or crystallite size) the most potent nanoparticles for use as reinforcement in a nanocomposite for advanced structural applications can be designed. Using the data of relevant mechanical properties generated by prior MD simulations for the most potent nanoparticles and those available in literature for the matrix phase, the FEM based tensile model has been formulated for nanocomposites. The multiscale model has been validated by the experimental data of Young's modulus obtained in the present work by nanoindentation testing of Al based Ni nanocomposites with different volume fraction loading of Ni nanoparticles. The FEM model based parametric study by altering the relevant parameters like volume fraction loading, size distribution and spatial distribution of the reinforcing nanoparticles within the nanocomposites; followed by an optimization analysis can lead to the design of most potent nanocomposite for advanced structural applications. The pre-designed target nanocomposite for advanced structural applications can be developed conveniently with minimum number of experimental trials. Thus, the scheme of multiscale modelling presented here can be very useful for the design and development of new promising nanocomposite materials for any advanced structural application.

Keywords: Multiscale Modelling and Simulations; Molecular Dynamics; Finite Element Method; Design and Development; Nanoparticles; Nanocomposites; Alloy Nanoparticles; Poly-nanocrystalline Alloy Thin Film; Tensile Model; Nanoindentation Model; Advanced Structural Materials.